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Supporting Information

V-Shaped Methylpyrimidinium Chromophores for Nonlinear Optics

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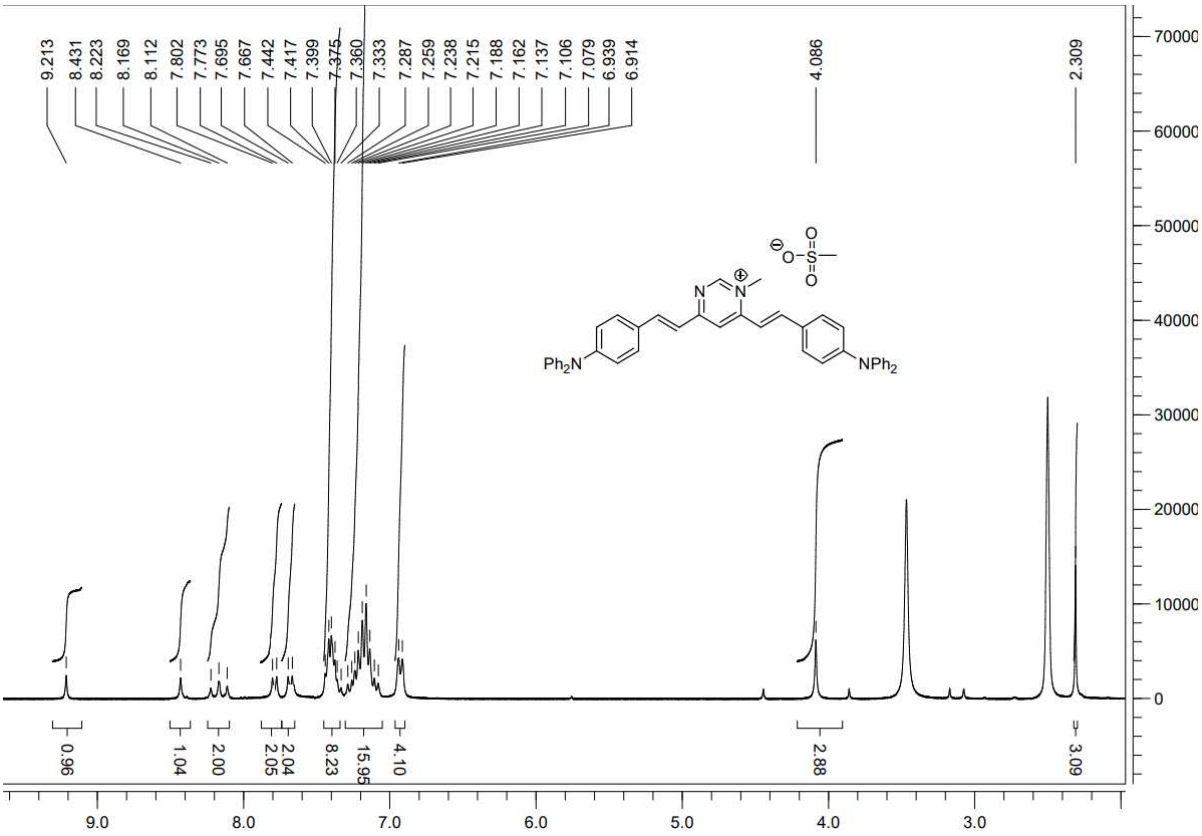


Figure S1 : ^{1}H NMR spectrum (300 MHz) of **1** in DMSO-d_6

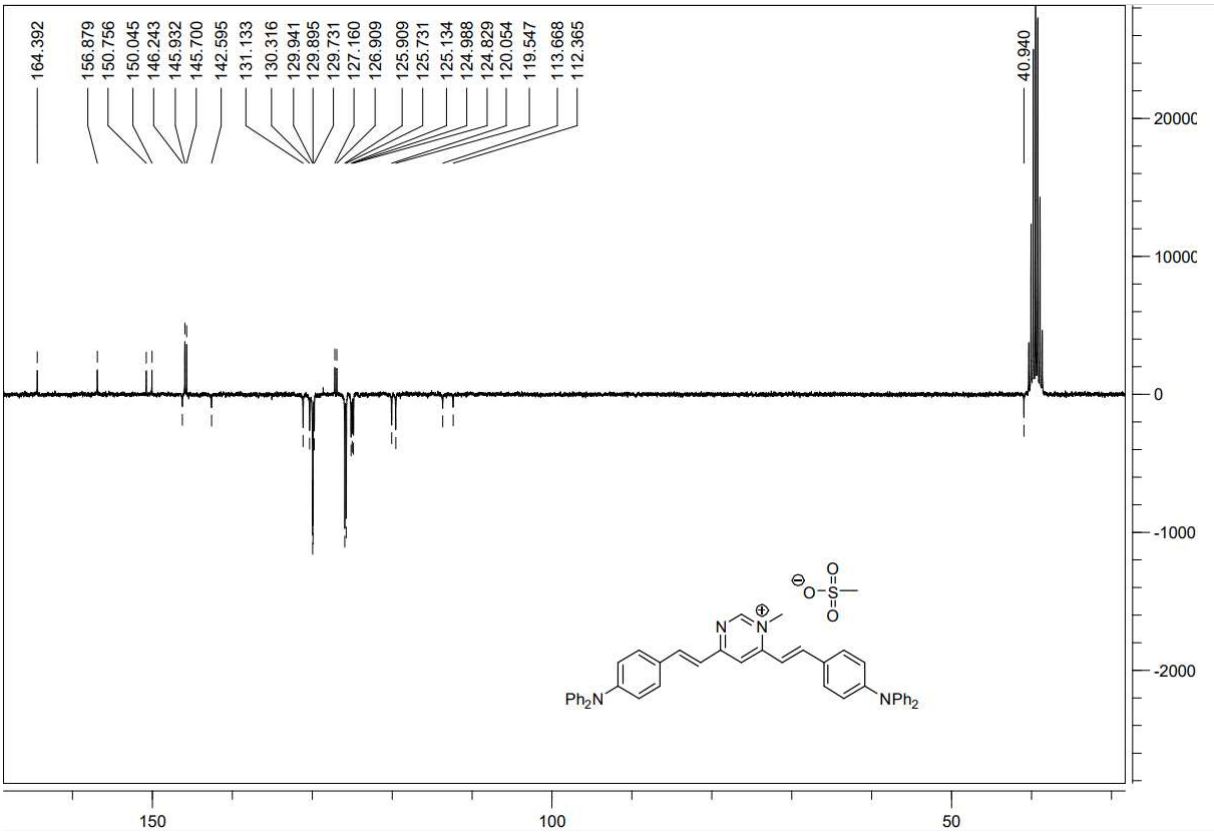


Figure S2 : ^{13}C NMR spectrum (75 MHz) of **1** in DMSO-d_6

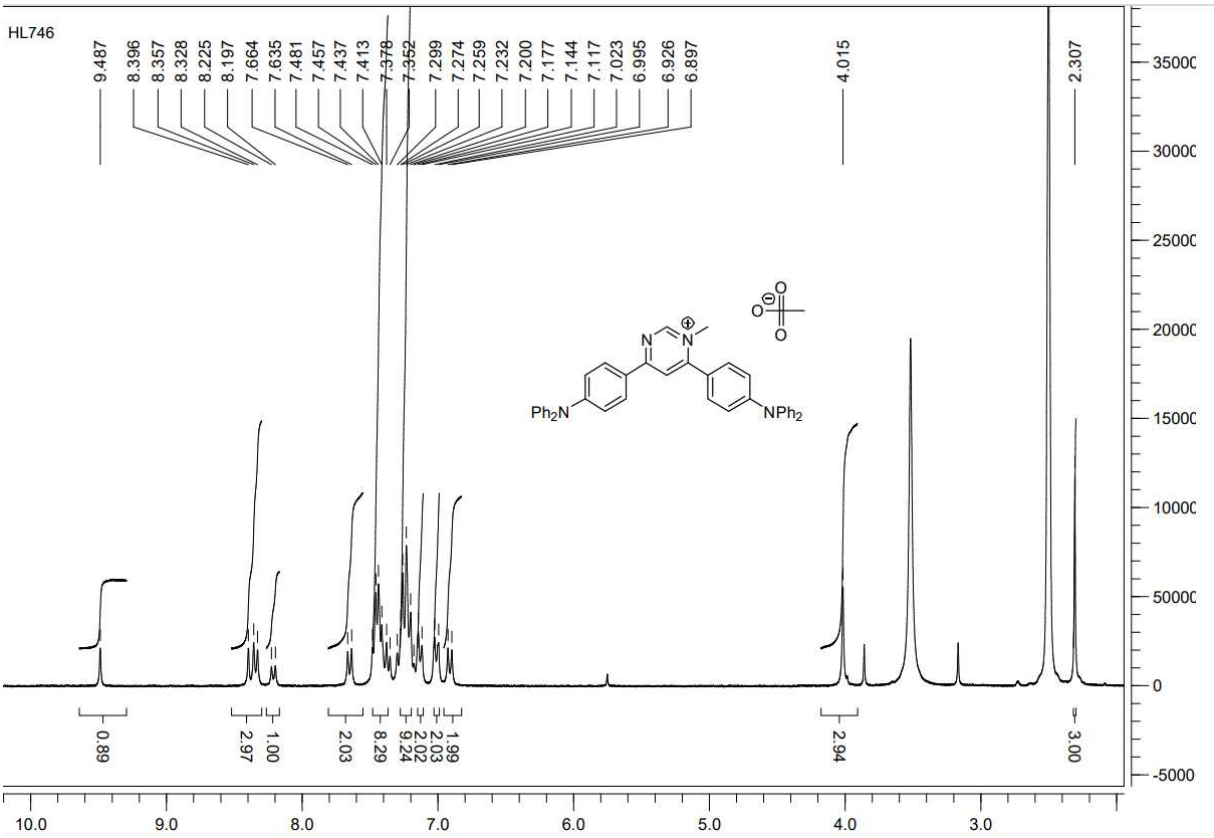


Figure S3 : ^{1}H NMR spectrum (300 MHz) of **2** in DMSO-d_6

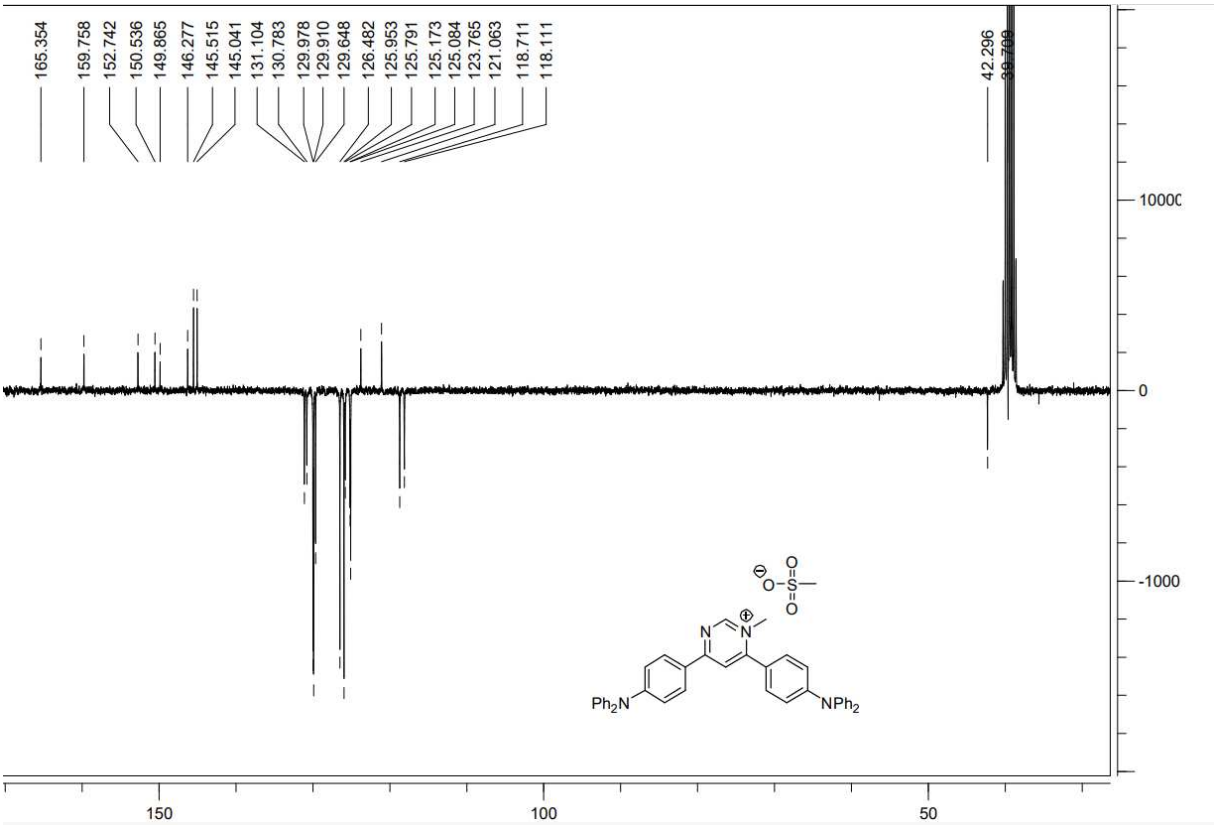


Figure S4 : ^{13}C NMR spectrum (75 MHz) of **2** in DMSO-d_6

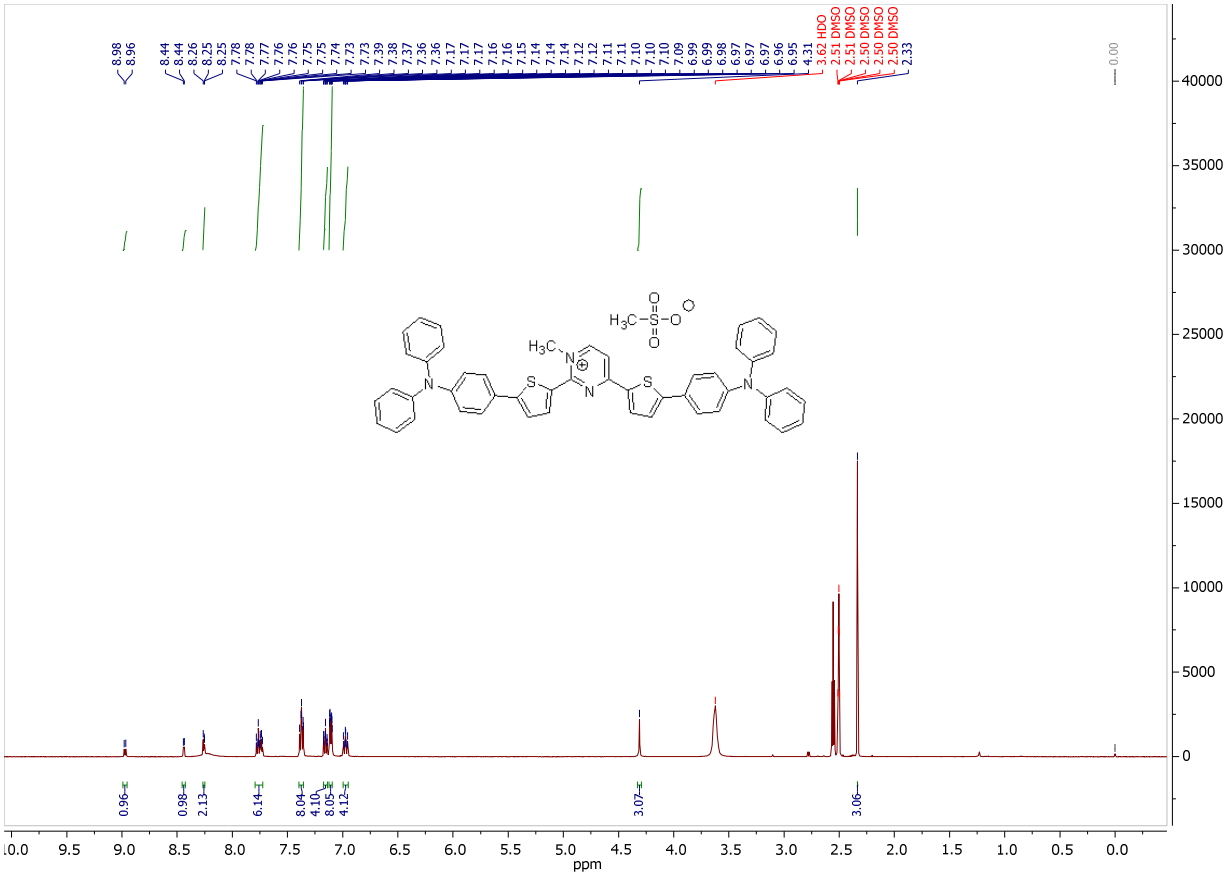


Figure S5 : ^{1}H NMR spectrum (500 MHz) of **3** in DMSO-d_6

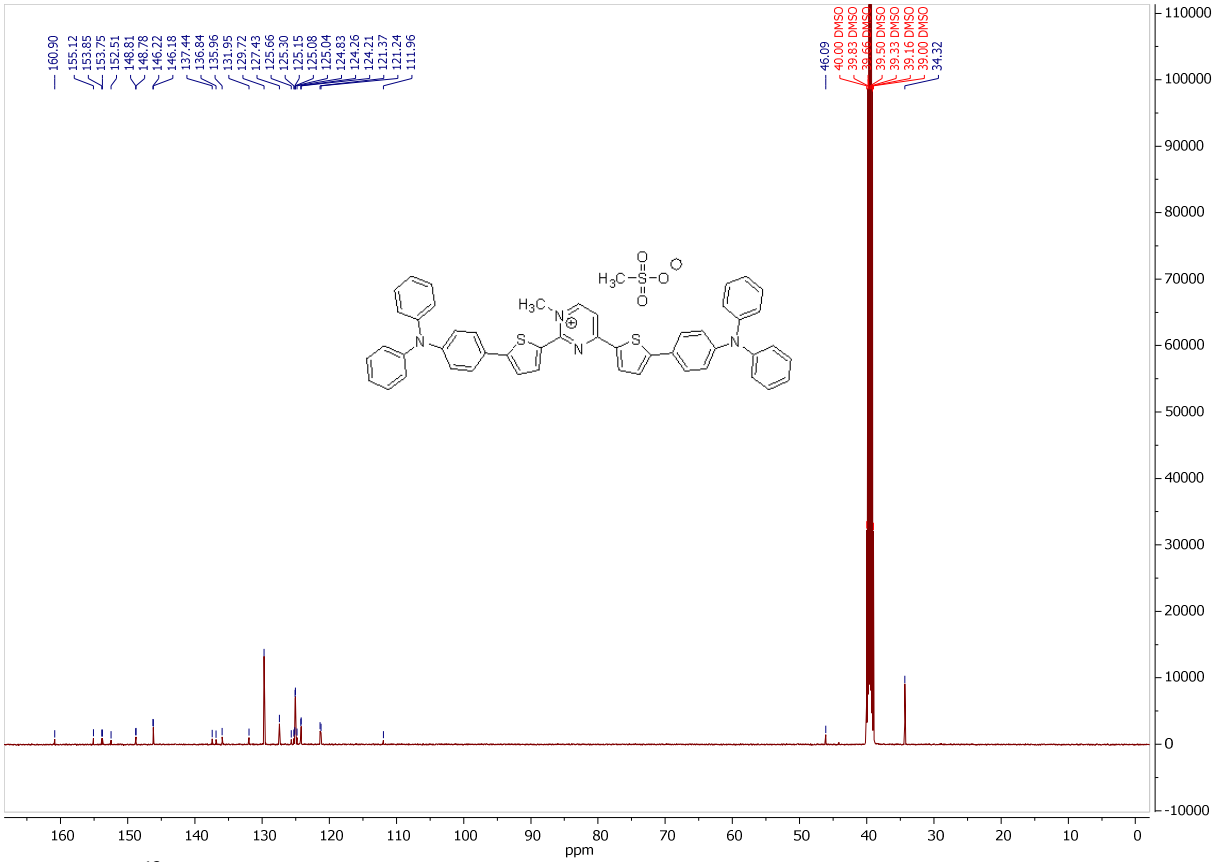


Figure S6 : ^{13}C NMR spectrum (125 MHz) of **3** in DMSO-d_6

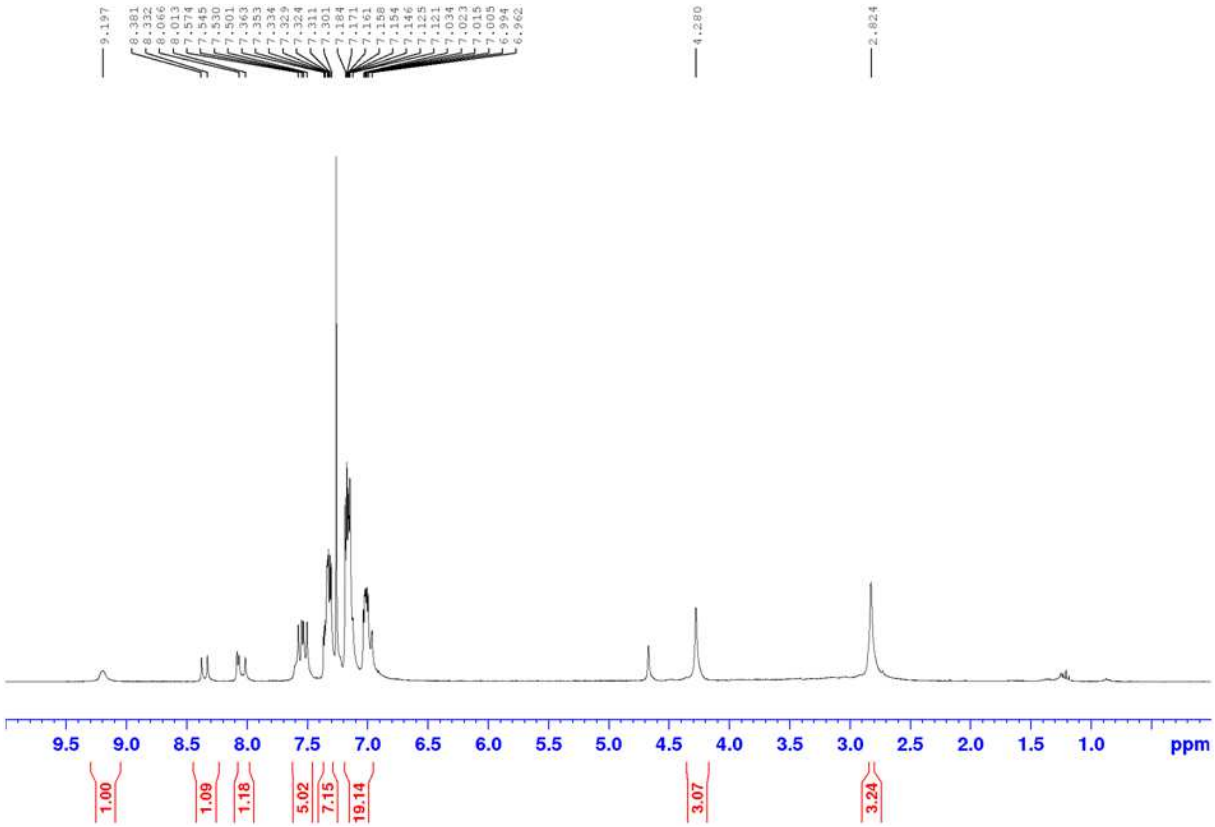


Figure S7 : ^{1}H NMR spectrum (300 MHz) of **4** in DMSO-d_6

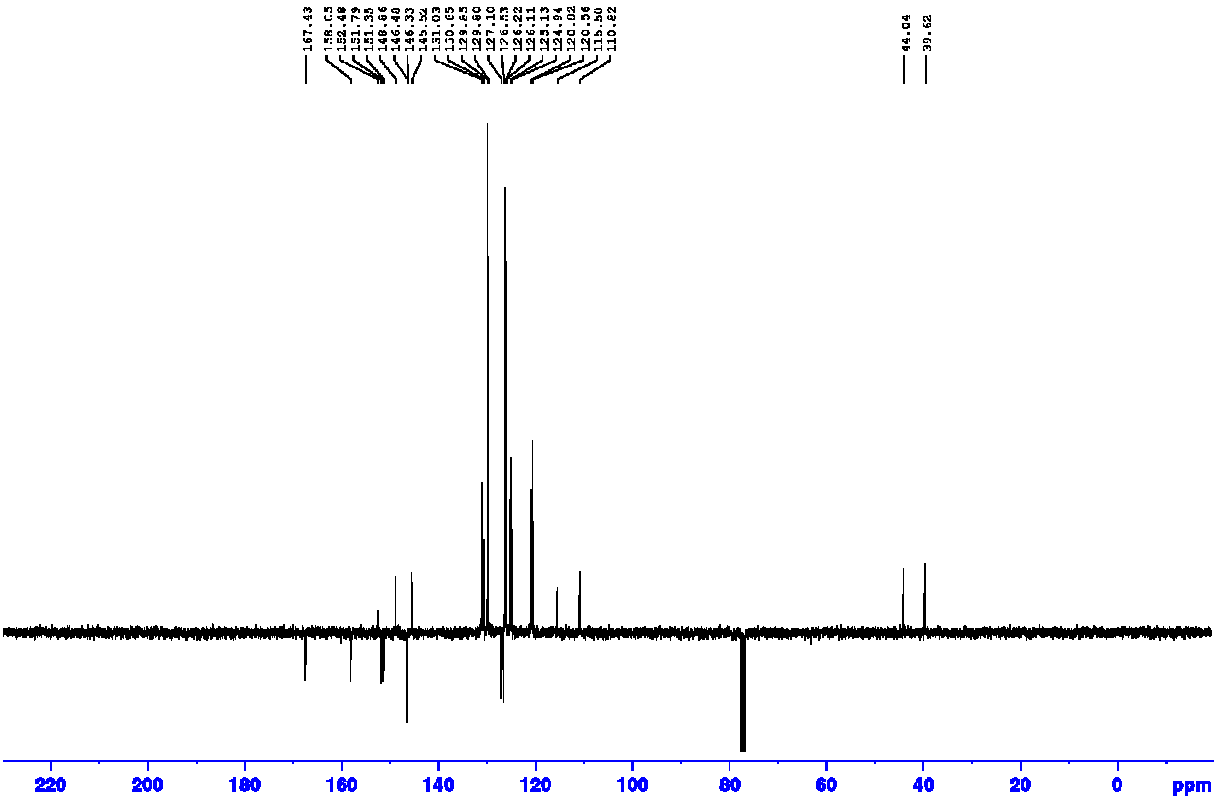
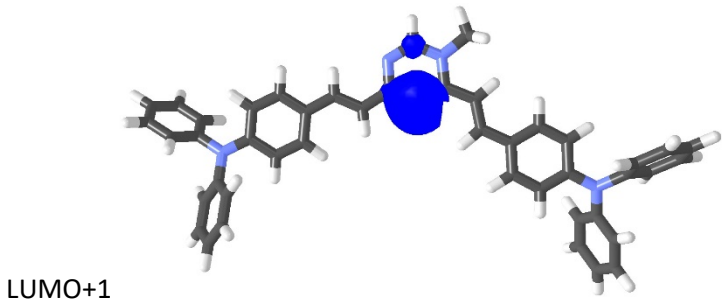
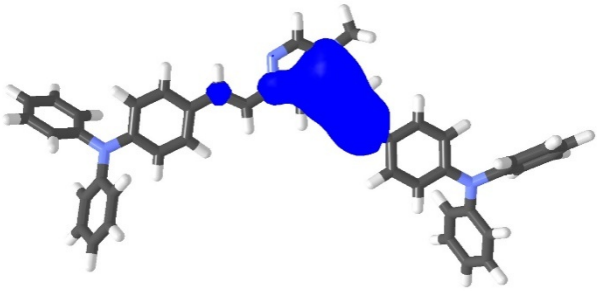


Figure S8 : ^{13}C NMR spectrum (75 MHz) of **4** in DMSO-d_6

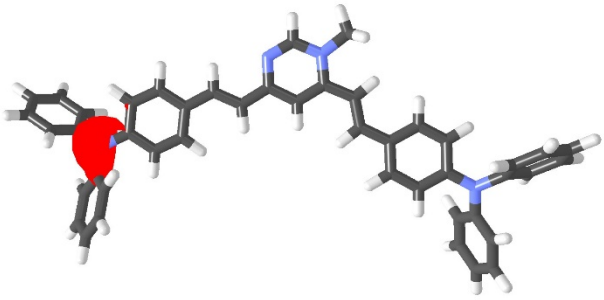
DFT calculations



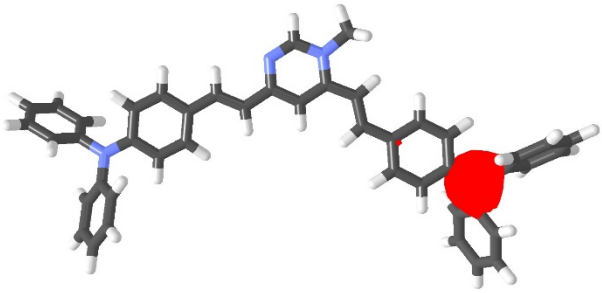
LUMO+1



LUMO

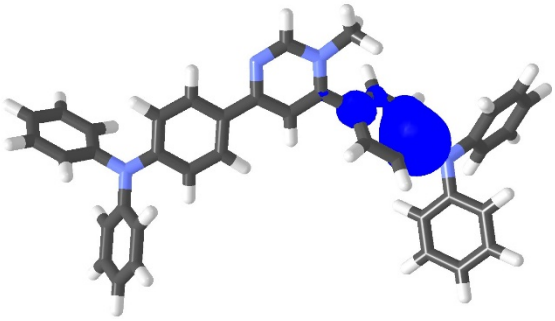


HOMO

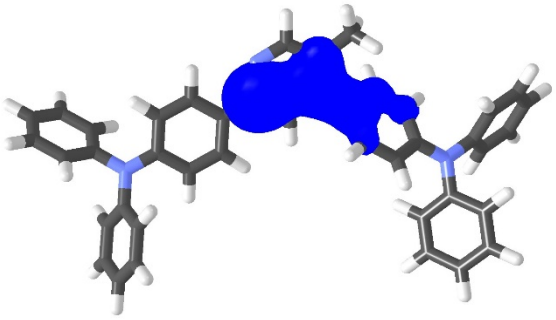


HOMO-1

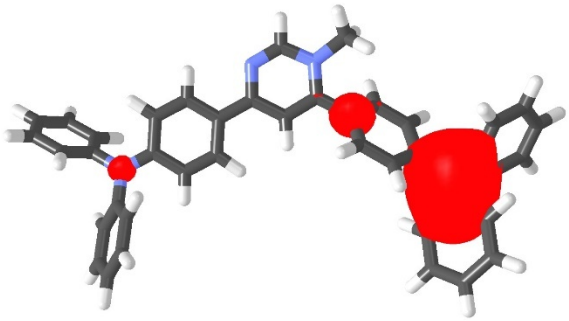
Figure S9 : HOMO(-1) and LUMO(+1) localizations in chromophore **1** shown in red and blue, respectively.



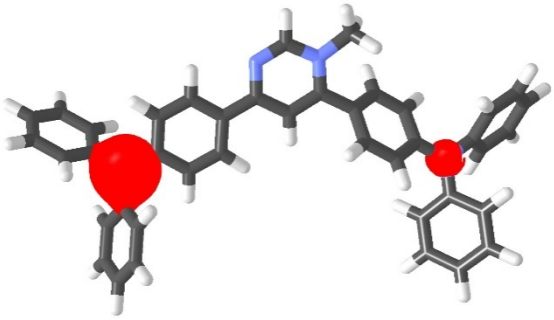
LUMO+1



LUMO

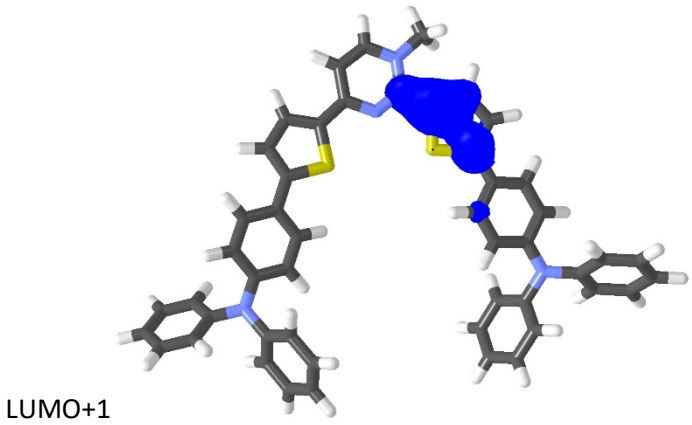


HOMO

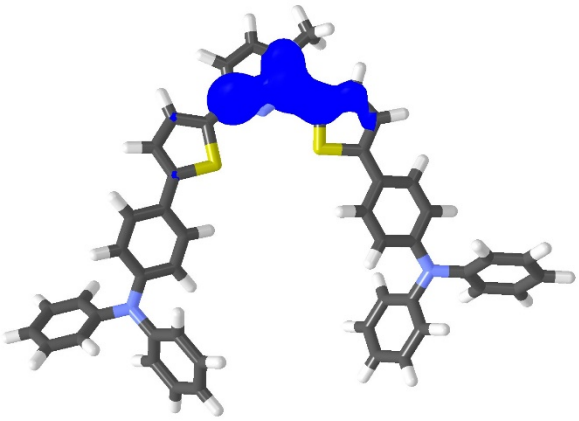


HOMO-1

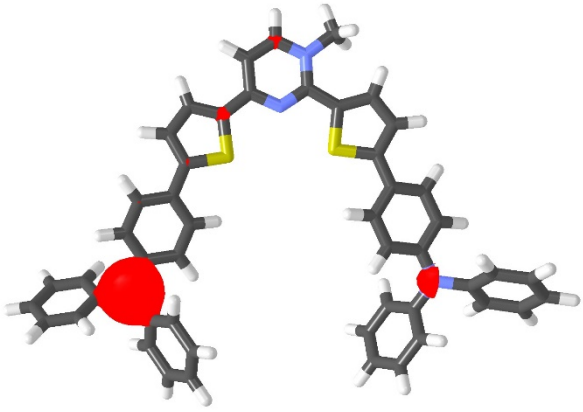
Figure S10 : HOMO(-1) and LUMO(+1) localizations in chromophore **2** shown in red and blue, respectively.



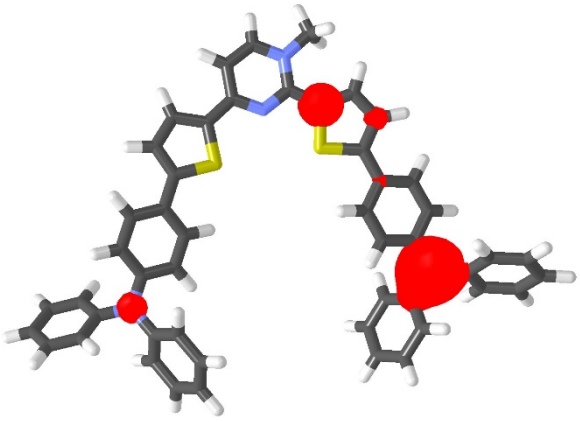
LUMO+1



LUMO

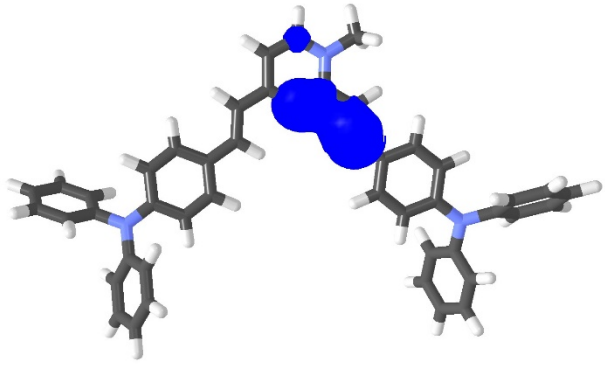


HOMO

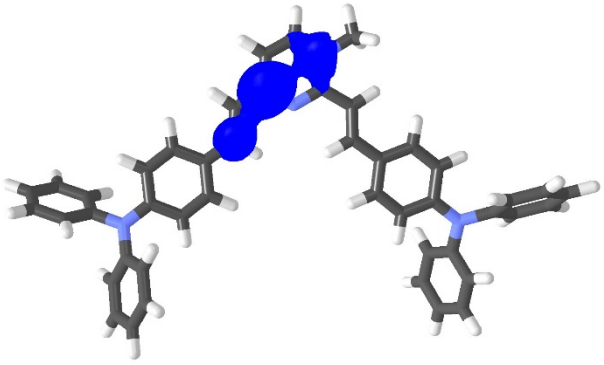


HOMO-1

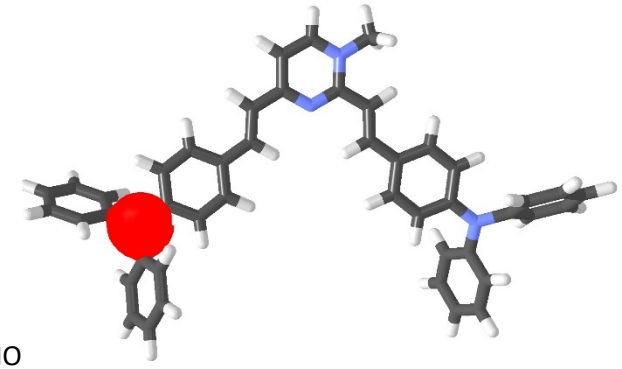
Figure S11 : HOMO(-1) and LUMO(+1) localizations in chromophore **3** shown in red and blue, respectively.



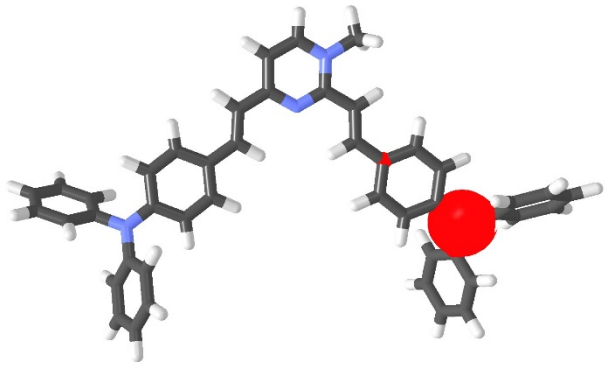
LUMO+1



LUMO



HOMO



HOMO-1

Figure S12 : HOMO(-1) and LUMO(+1) localizations in chromophore **4** shown in red and blue, respectively.

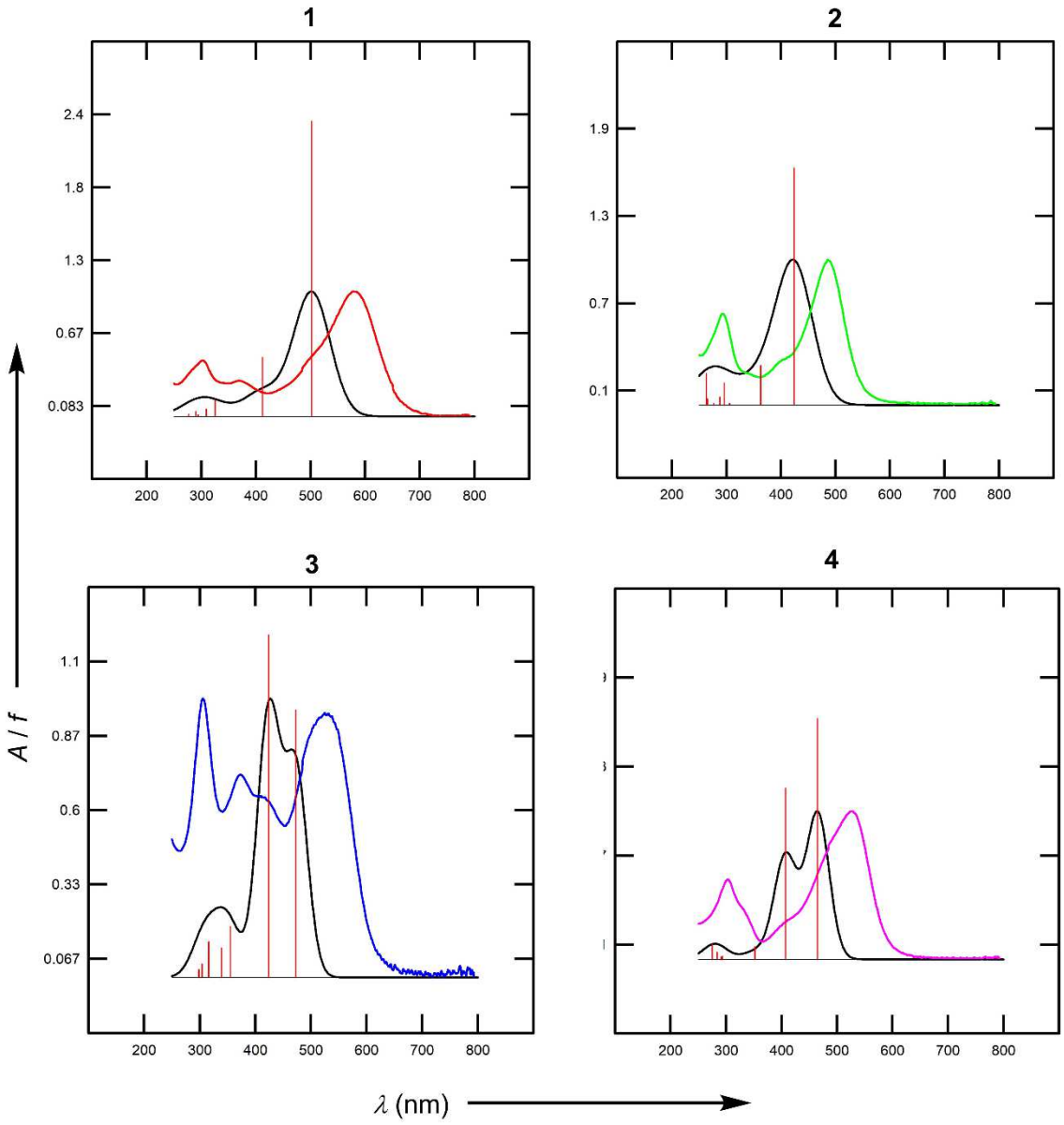


Figure S13 : TD-DFT (n states = 8) CAM-B3LYP/6-311+G(2df,p) calculated UV-Vis spectra of chromophores **1**-**4** (black) along with the experimentally obtained spectra (in color) in $CHCl_3$. Red vertical lines represent oscillator strengths (*f*).

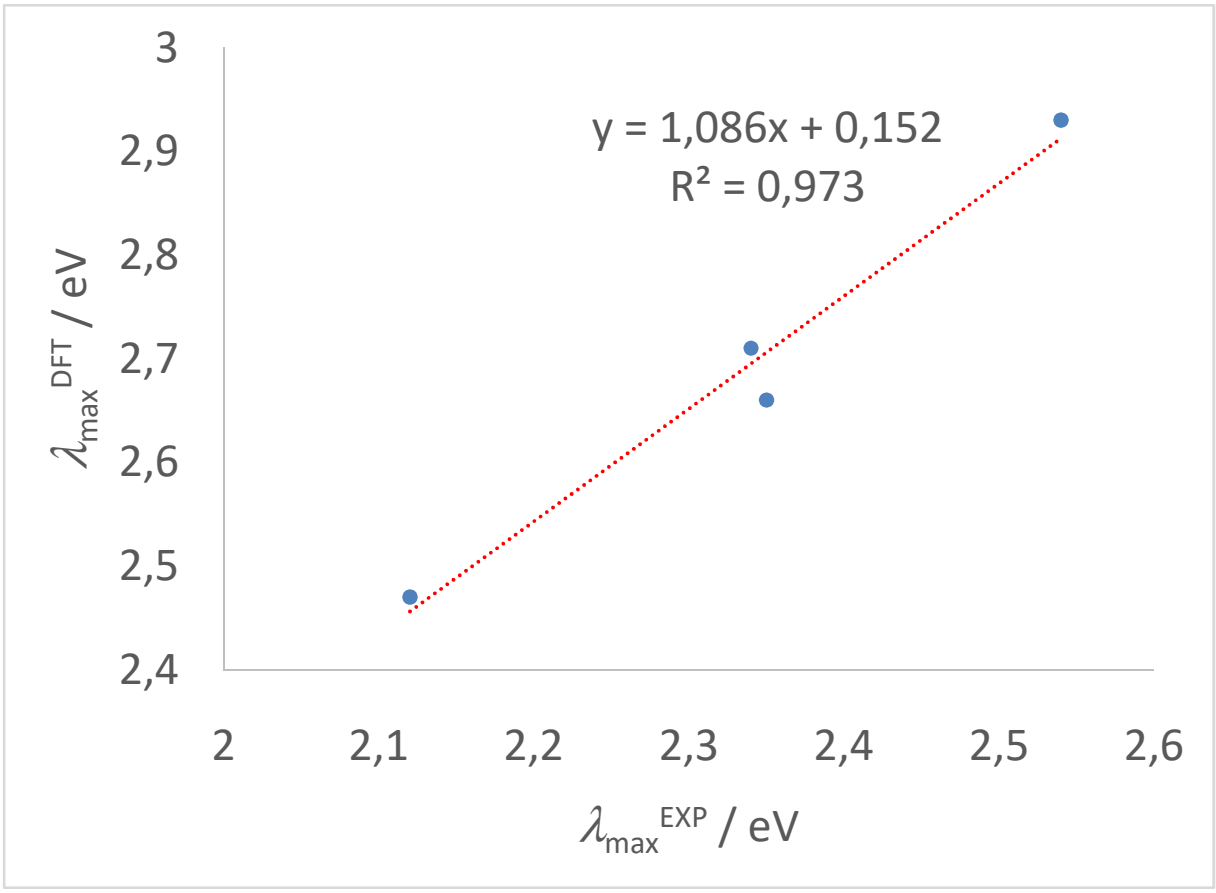


Figure S14 : Correlation of TD-DFT calculated and experimental longest-wavelength absorption maxima λ_{max}.